

FIG. 1A

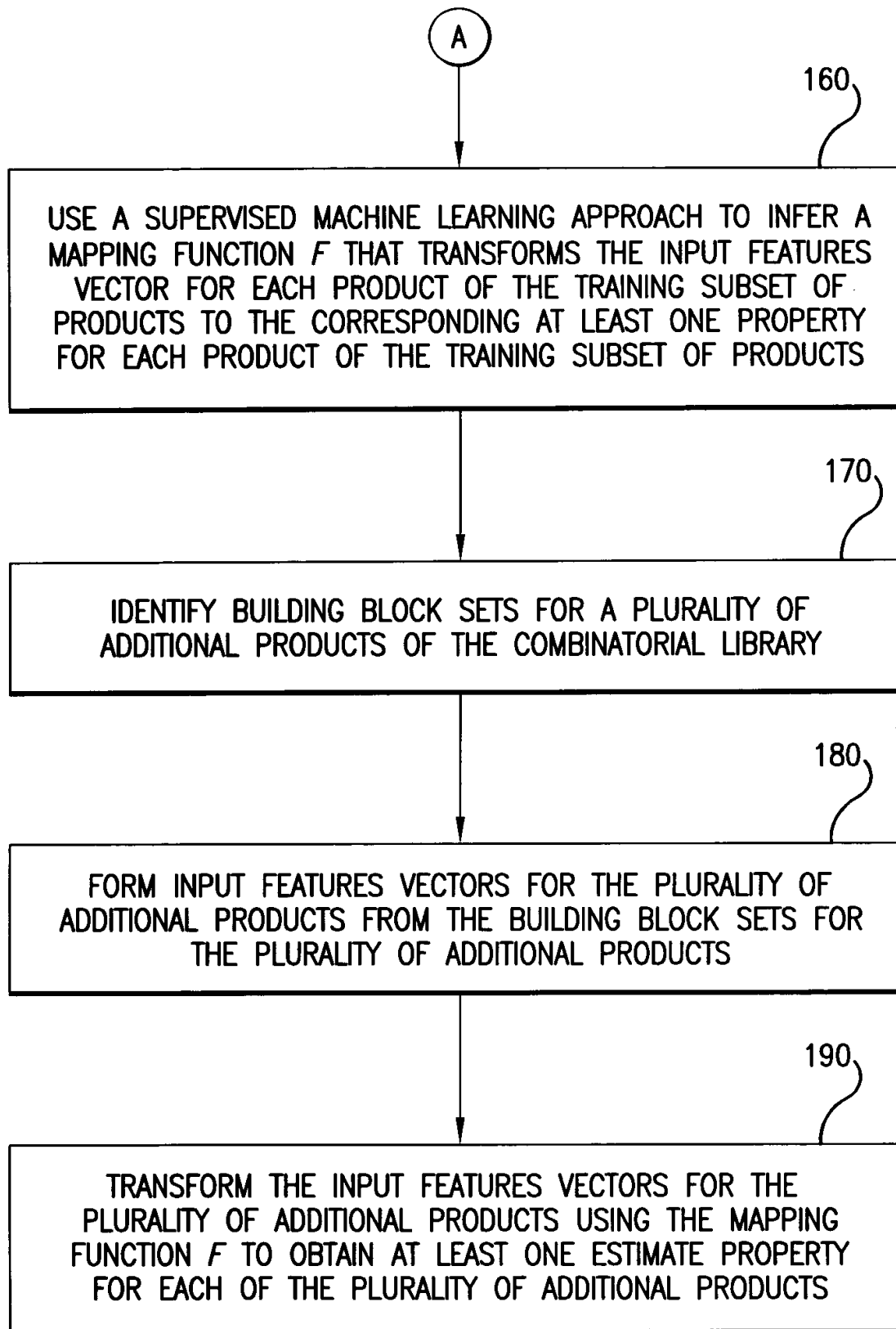


FIG. 1B

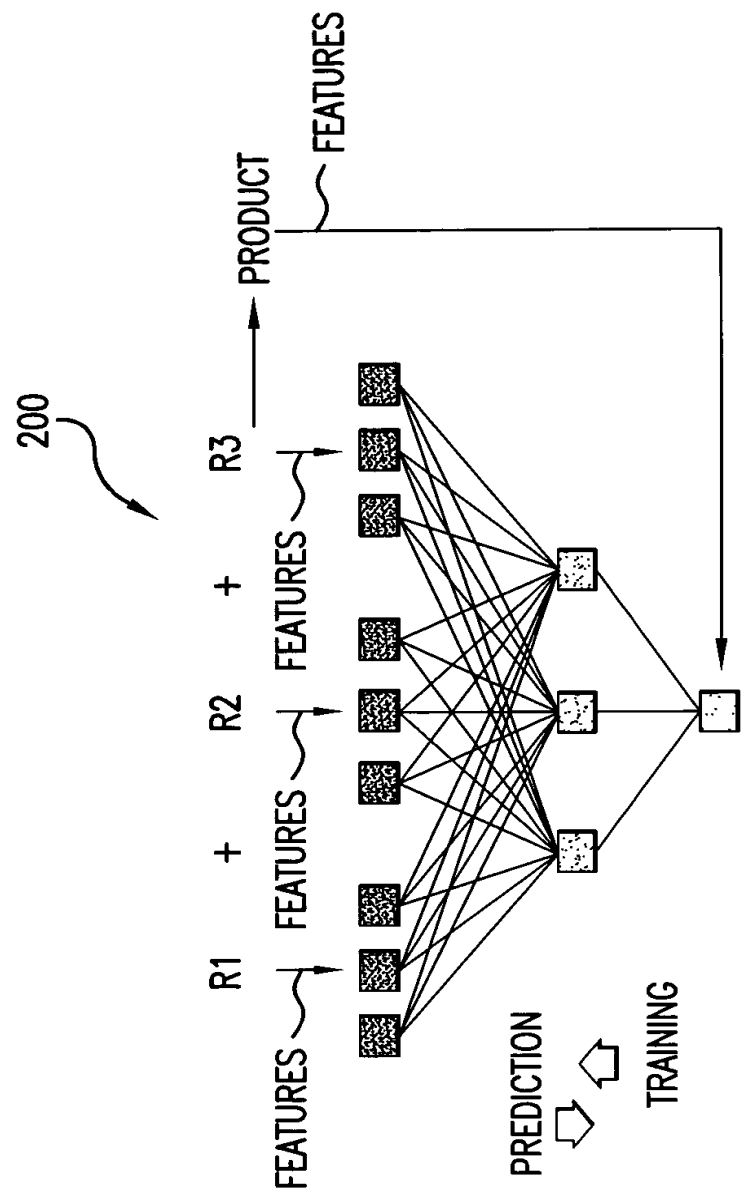


FIG.2

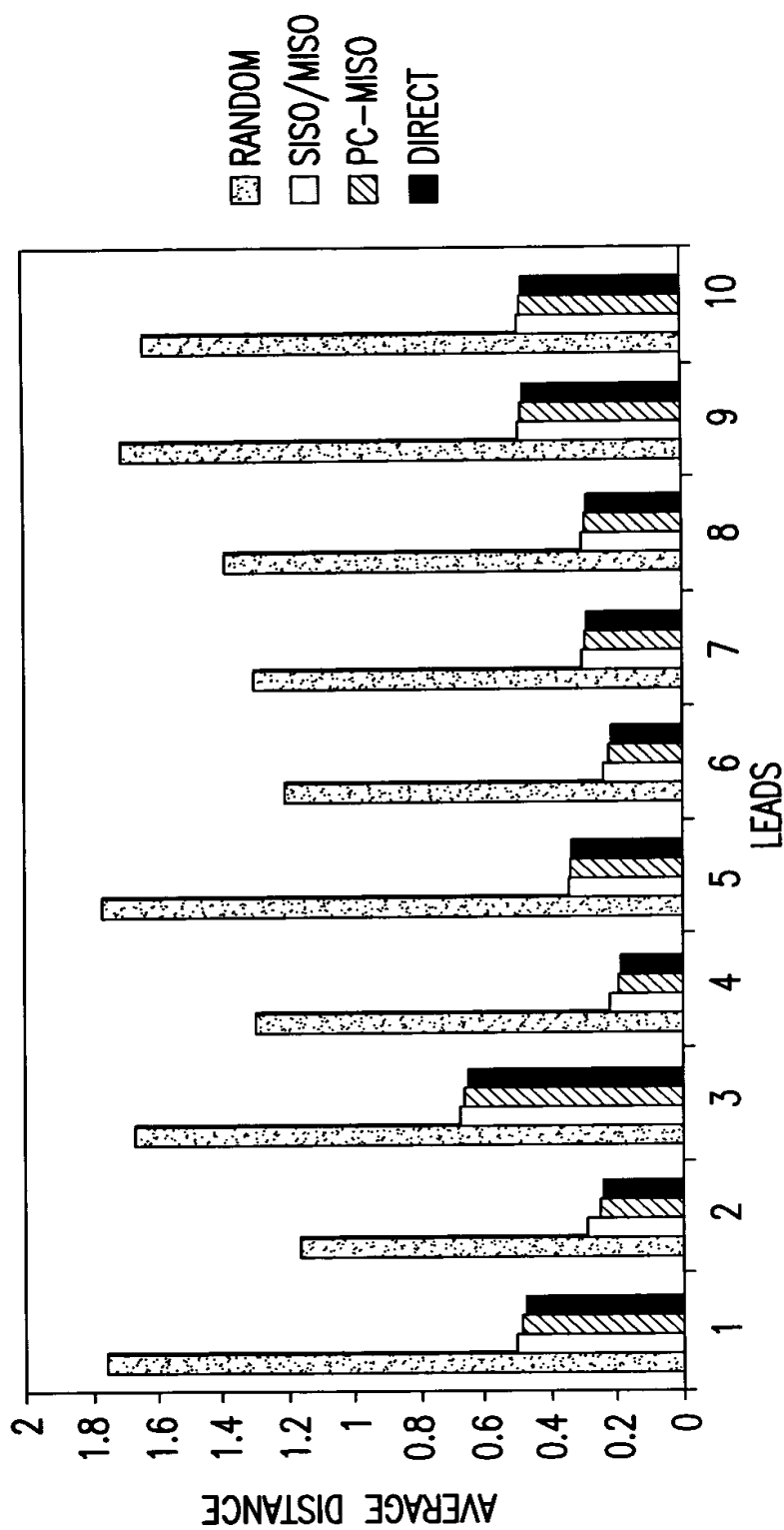


FIG. 3

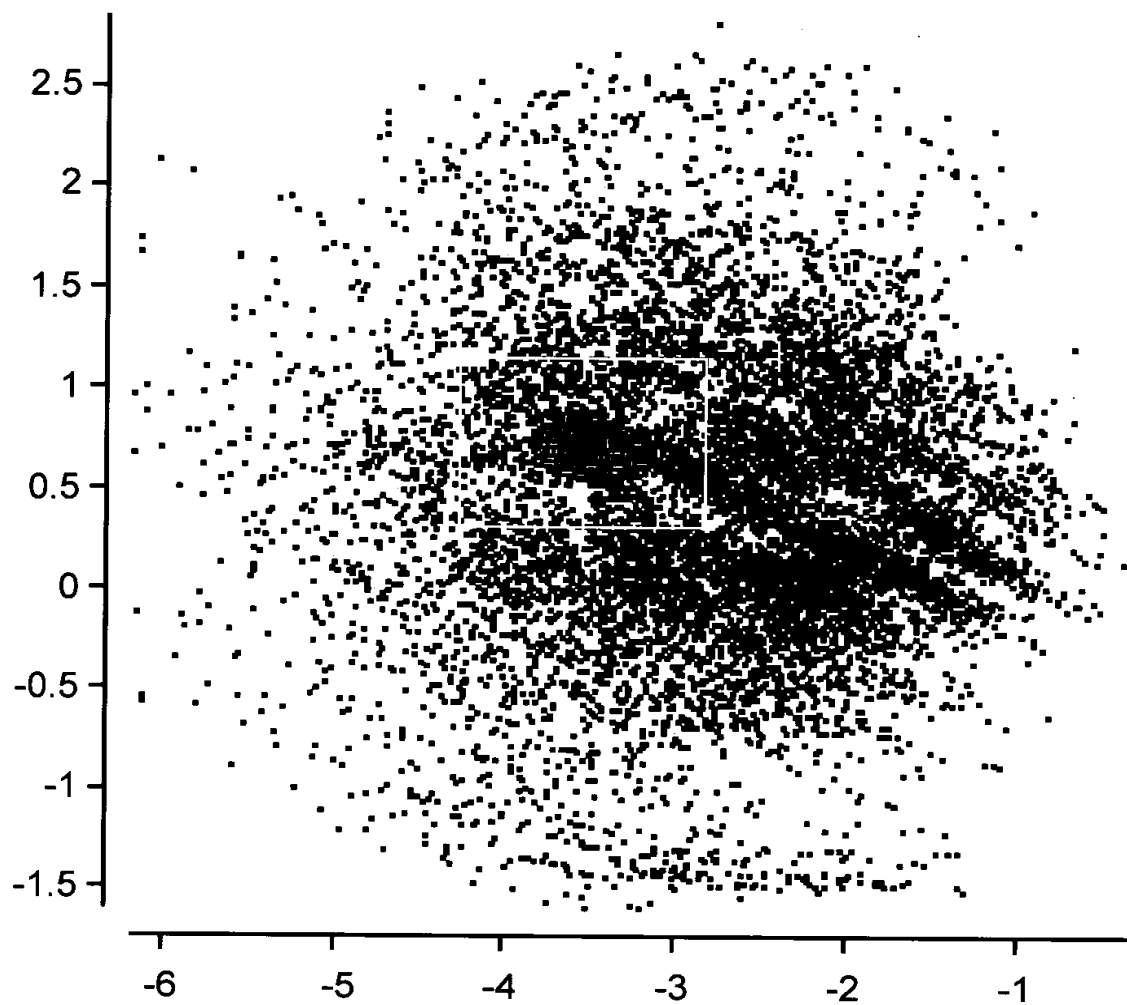


FIG.4A

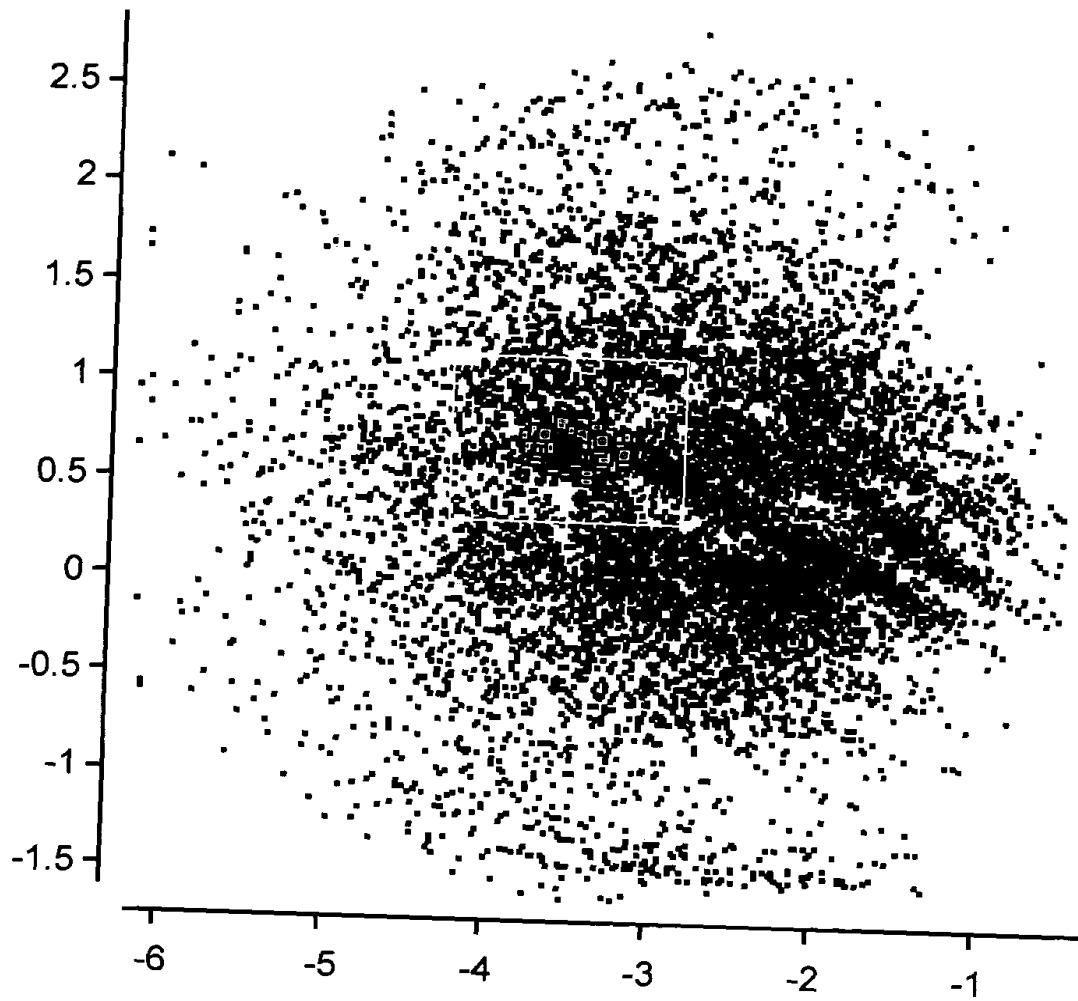


FIG.4B

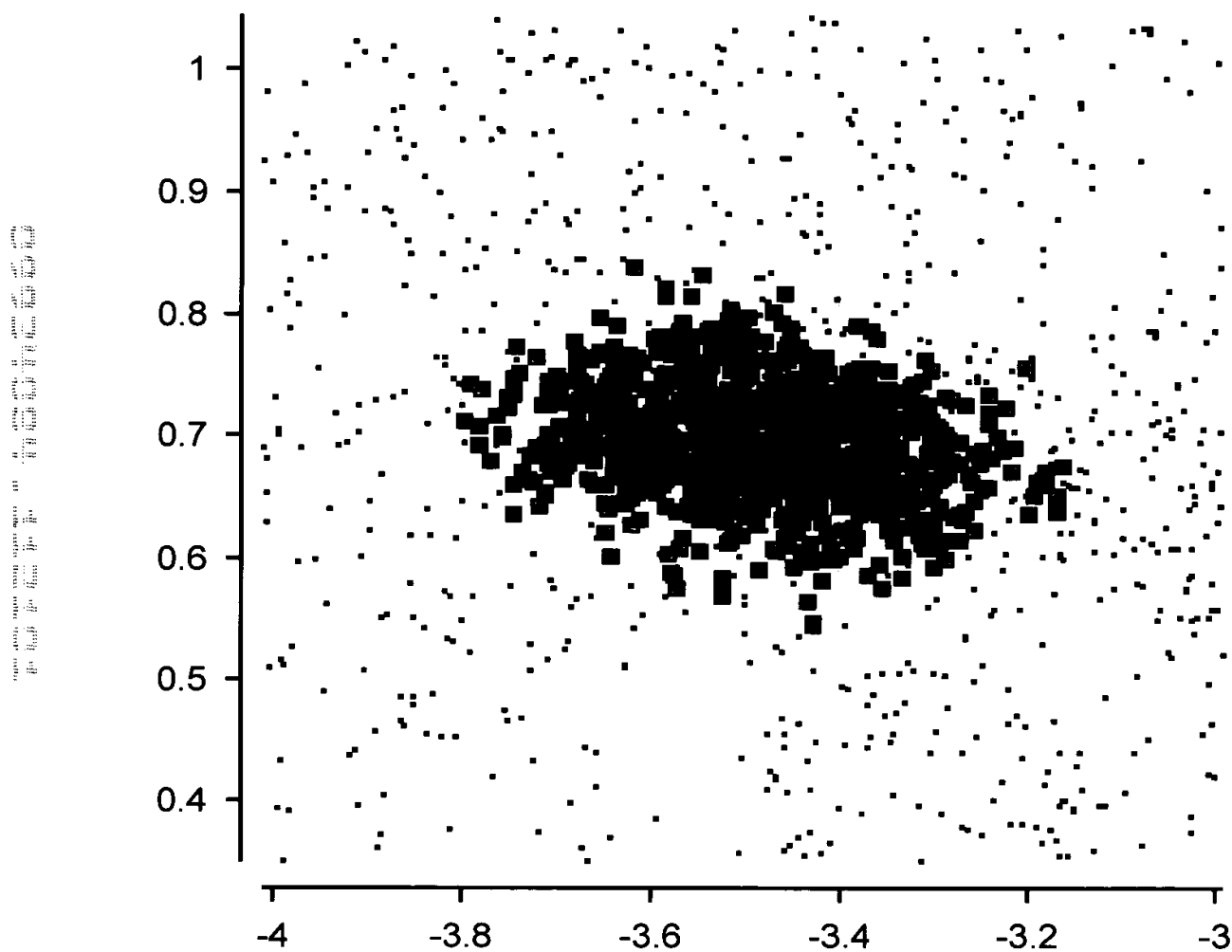


FIG.4C

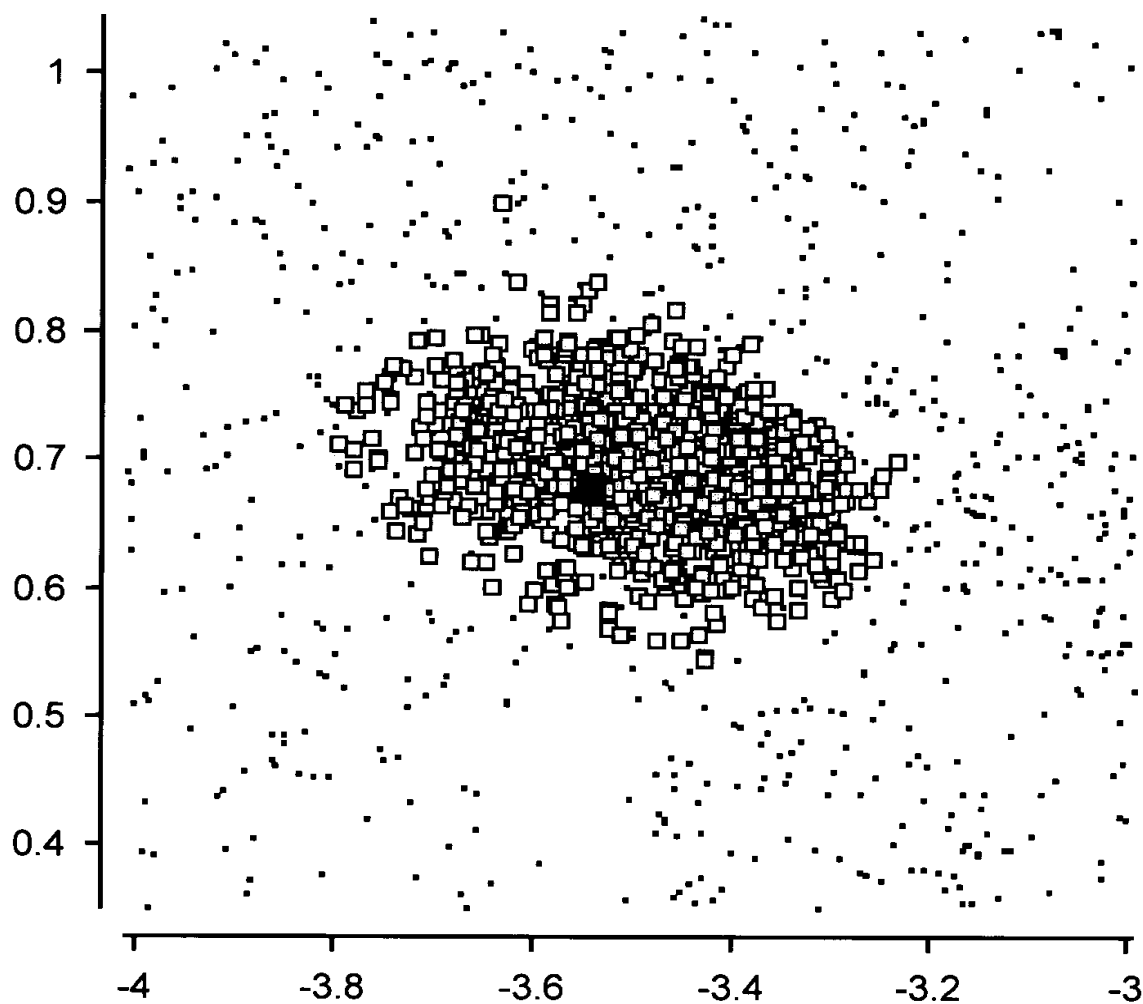
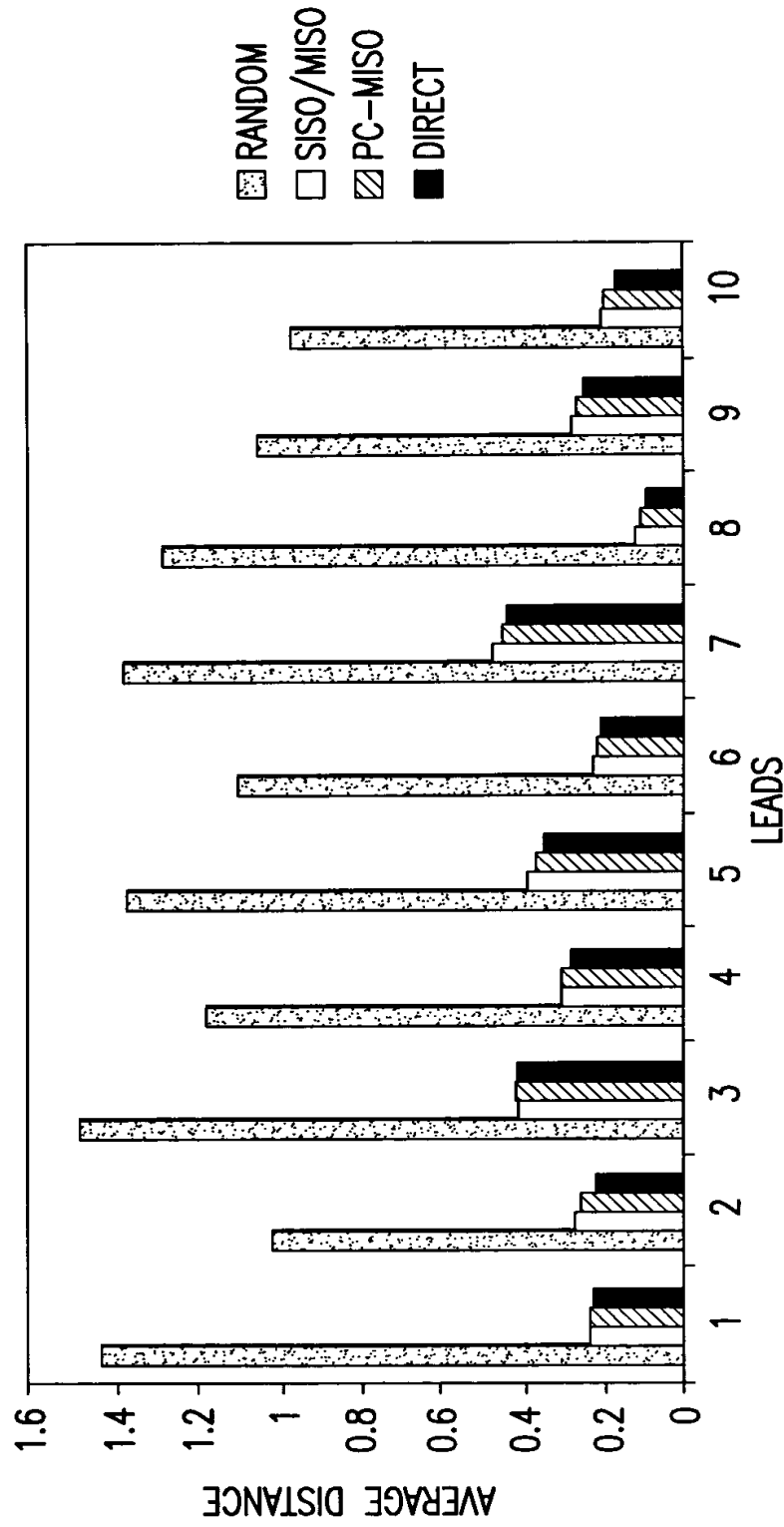


FIG.4D





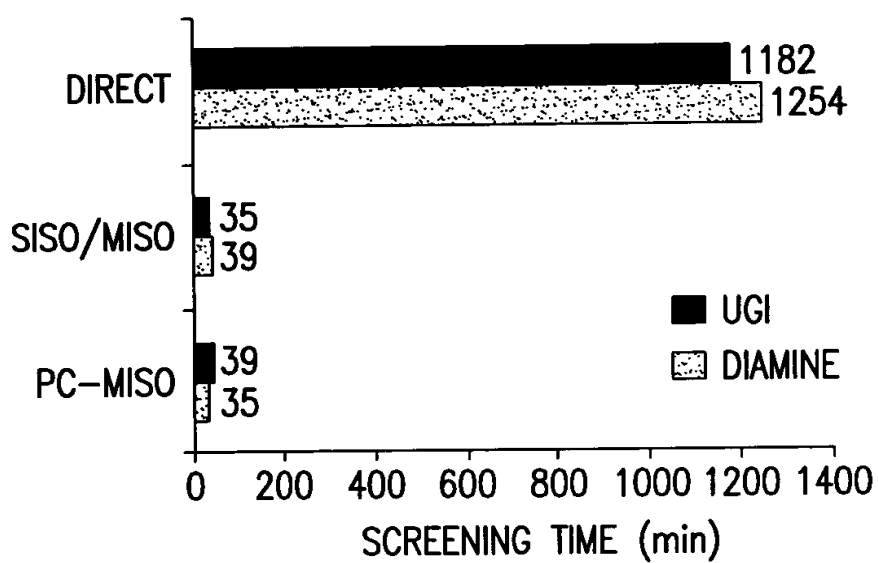


FIG.6

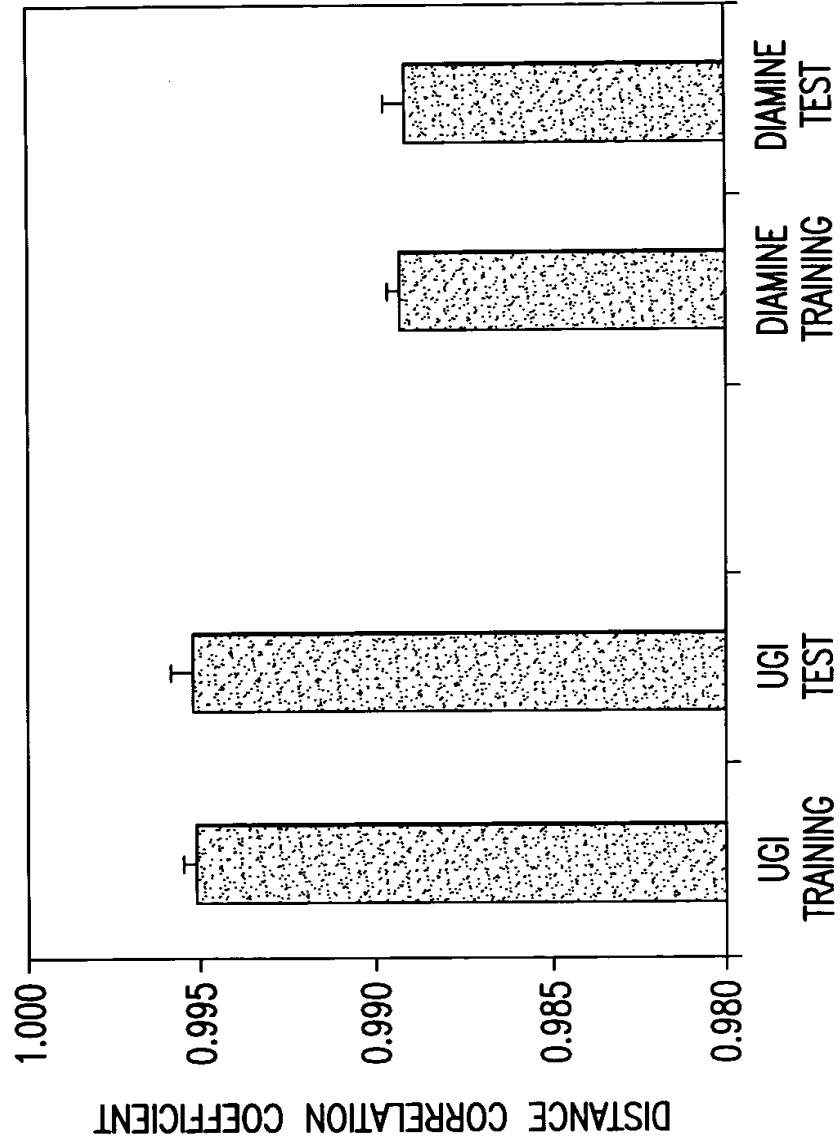


FIG. 7

USPTO OFFICE ACTION NO. 09/934,084; GROUP ART UNIT: 2857  
Dkt. No. 1503.1070003; Batch No.: N/A  
Inventor(s): Lobanov et al.; Tel: 202/371-2600  
Title: Method, System, and Computer Program Product for  
Determining Properties of Combinatorial Library Products...

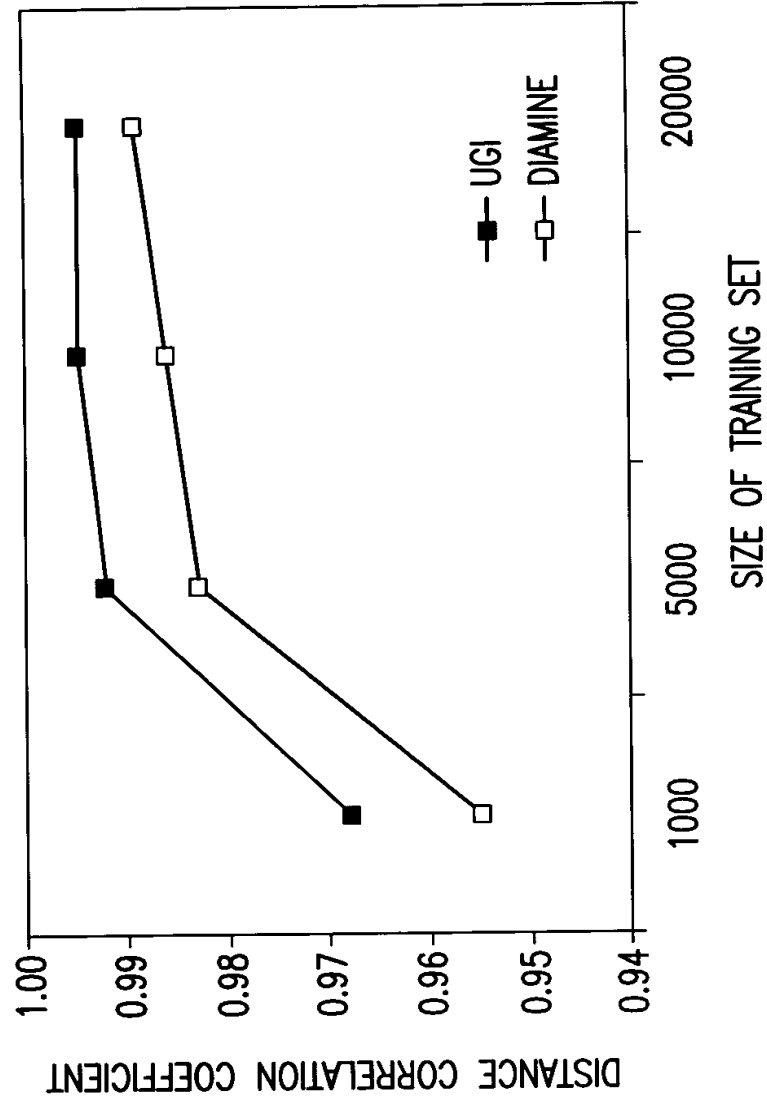


FIG.8

FIG. 8 is a line graph showing the Distance Correlation Coefficient (Y-axis, ranging from 0.94 to 1.00) versus the Size of Training Set (X-axis, ranging from 1000 to 20000). Two datasets are compared: UCI (represented by a solid line with square markers) and DIAMINE (represented by a dashed line with open square markers). Both datasets show an increasing trend in the Distance Correlation Coefficient as the training set size increases. The UCI dataset consistently shows a higher Distance Correlation Coefficient than the DIAMINE dataset for the same training set size.

INDEX	DESCRIPTOR	SISO TRAINING R <sup>2</sup>	SISO TEST R <sup>2</sup>	MISO TRAINING R <sup>2</sup>	MISO TEST R <sup>2</sup>
1	NO. ATOMS	0.996	0.997		
2	NO. BONDS	0.995	0.996		
3	NO. ELEMENTS	0.603	0.614	0.822	0.823
4	MOLECULAR WEIGHT	0.996	0.997		
5	CHI 0	0.996	0.997		
6	CHI PATH 1	0.996	0.997		
7	CHI PATH 2	0.994	0.995		
8	CHI PATH 3	0.971	0.973		
9	CHI PATH 4	0.974	0.976		
10	CHI PATH 5	0.956	0.957		
11	CHI PATH 6	0.909	0.910		
12	CHI PATH 7	0.837	0.843	0.943	0.942
13	CHI PATH 8	0.666	0.673	0.938	0.934
14	CHI PATH 9	0.563	0.554	0.939	0.936
15	CHI PATH 10	0.447	0.457	0.950	0.950
16	CHI CLUSTER 3	0.988	0.987		
17	CHI CLUSTER 4	0.993	0.993		
18	CHI PATH/CLUSTER 4	0.978	0.980		
19	VAL CHI 0	0.996	0.997		
20	VAL CHI PATH 1	0.997	0.998		
21	VAL CHI PATH 2	0.996	0.996		
22	VAL CHI PATH 3	0.993	0.994		
23	VAL CHI PATH 4	0.981	0.982		
24	VAL CHI PATH 5	0.952	0.951		
25	VAL CHI PATH 6	0.907	0.905		

FIG. 9A

INDEX	DESCRIPTOR	SISO TRAINING R <sup>2</sup>	SISO TEST R <sup>2</sup>	MISO TRAINING R <sup>2</sup>	MISO TEST R <sup>2</sup>
26	VAL CHI PATH 7	0.773	0.775	0.901	0.905
27	VAL CHI PATH 8	0.619	0.621	0.890	0.889
28	VAL CHI PATH 9	0.349	0.328	0.910	0.910
29	VAL CHI PATH 10	0.222	0.201	0.921	0.920
30	VAL CHI CLUSTER 3	0.994	0.994		
31	VAL CHI CLUSTER 4	0.993	0.993		
32	VAL CHI PATH/CLUSTER 4	0.988	0.989		
33	CHI CHAIN 3	1.000	1.000		
34	CHI CHAIN 4	1.000	1.000		
35	CHI CHAIN 5	0.979	0.978		
36	CHI CHAIN 6	0.995	0.995		
37	CHI CHAIN 7	0.999	0.999		
38	CHI CHAIN 8	1.000	1.000		
39	CHI CHAIN 9	0.999	0.999		
40	CHI CHAIN 10	0.999	0.998		
41	VAL CHI CHAIN 3	1.000	1.000		
42	VAL CHI CHAIN 4	1.000	1.000		
43	VAL CHI CHAIN 5	0.994	0.996		
44	VAL CHI CHAIN 6	0.994	0.995		
45	VAL CHI CHAIN 7	0.998	0.998		
46	VAL CHI CHAIN 8	1.000	1.000		
47	VAL CHI CHAIN 9	0.997	0.998		
48	VAL CHI CHAIN 10	0.986	0.980		
49	SUBGRAPH COUNT PATH 2	0.996	0.997		
50	SUBGRAPH COUNT PATH 3	0.990	0.990		

FIG. 9B

INDEX	DESCRIPTOR	SISO TRAINING R <sup>2</sup>	SISO TEST R <sup>2</sup>	MISO TRAINING R <sup>2</sup>	MISO TEST R <sup>2</sup>
51	SUBGRAPH COUNT PATH 4	0.957	0.960		
52	SUBGRAPH COUNT PATH 5	0.914	0.918		
53	SUBGRAPH COUNT PATH 6	0.837	0.844	0.909	0.905
54	SUBGRAPH COUNT PATH 7	0.752	0.770	0.892	0.887
55	SUBGRAPH COUNT PATH 8	0.582	0.599	0.907	0.906
56	SUBGRAPH COUNT PATH 9	0.446	0.448	0.933	0.932
57	SUBGRAPH COUNT PATH 10	0.366	0.383	0.947	0.945
58	SUBGRAPH COUNT CLUSTER 3	0.994	0.995		
59	SUBGRAPH COUNT CLUSTER 4	0.991	0.991		
60	SUBGRAPH COUNT PATH/CLUSTER 4	0.980	0.980		
61	SUBGRAPH COUNT RING 3	1.000	1.000		
62	SUBGRAPH COUNT RING 4	1.000	1.000		
63	SUBGRAPH COUNT RING 5	0.995	0.995		
64	SUBGRAPH COUNT RING 6	0.994	0.995		
65	SUBGRAPH COUNT RING 7	1.000	1.000		
66	SUBGRAPH COUNT RING 8	1.000	1.000		
67	SUBGRAPH COUNT RING 9	1.000	1.000		
68	SUBGRAPH COUNT RING 10	0.999	0.999		
69	KAPPA 0	0.980	0.980		
70	KAPPA 1	0.991	0.992		
71	KAPPA 2	0.907	0.908		
72	KAPPA 3	0.709	0.710	0.806	0.799
73	KAPPA ALPHA 1	0.987	0.987		
74	KAPPA ALPHA 2	0.895	0.897	0.960	0.955
75	KAPPA ALPHA 3	0.685	0.686	0.774	0.770

FIG. 9C

INDEX	DESCRIPTOR	SISO TRAINING R <sup>2</sup>	SISO TEST R <sup>2</sup>	MISO TRAINING R <sup>2</sup>	MISO TEST R <sup>2</sup>
76	WIENER PATH NO.	0.967	0.965		
77	TOTAL WIENER PATH NO.	0.903	0.892		
78	SHANNON INDEX	0.911	0.911		
79	TOTAL NO. OF PATHS	0.939	0.932		
80	BONCHEV-TRINAJSTIĆ IdW INDEX	0.958	0.955		
81	BONCHEV-TRINAJSTIĆ MEAN IdW INDEX	0.972	0.972		
82	BONCHEV-TRINAJSTIĆ IdC INDEX	0.979	0.978		
83	BONCHEV-TRINAJSTIĆ MEAN IdC INDEX	0.793	0.773	0.707	0.759
84	WIENER PARITY NO.	0.988	0.989		
85	PLATT F NO.	0.996	0.997		
86	DELTA PARTITION 1	0.996	0.996		
87	DELTA PARTITION 2	0.992	0.992		
88	DELTA PARTITION 3	0.997	0.997		
89	DELTA PARTITION 4	0.995	0.996		
90	DELTA PARTITION 5	1.000	1.000		
91	DELTA PARTITION 6	1.000	1.000		
92	NO. H	0.996	0.997		
93	NO. B	1.000	1.000		
94	No. C	0.997	0.998		
95	No. N	0.995	0.995		
96	No. O	0.994	0.993		
97	No. F	0.996	0.996		
98	No. Si	1.000	1.000		
99	No. P	0.999	0.999		

FIG. 9D



INDEX	DESCRIPTOR	SISO TRAINING R <sup>2</sup>	SISO TEST R <sup>2</sup>	MISO TRAINING R <sup>2</sup>	MISO TEST R <sup>2</sup>
100	No. S	0.997	0.999		
101	No. Cl	0.997	0.997		
102	No. Ge	1.000	1.000		
103	No. As	1.000	1.000		
104	No. Se	1.000	1.000		
105	No. Br	1.000	1.000		
106	No. I	1.000	1.000		
107	NO. HALOGENS	0.997	0.998		
108	TOTAL TOPOLOGICAL STATE 1	0.924	0.918		
109	TOTAL TOPOLOGICAL STATE 2	0.947	0.945		
110	TOTAL TOPOLOGICAL STATE 3	0.904	0.888		
111	TOTAL TOPOLOGICAL STATE 4	0.956	0.956		
112	TOTAL TOPOLOGICAL STATE 5	0.852	0.826	0.915	0.907
113	TOTAL TOPOLOGICAL STATE 6	0.980	0.980		
114	TOTAL TOPOLOGICAL STATE 7	0.832	0.790	0.914	0.889
115	TOTAL TOPOLOGICAL STATE 8	0.988	0.988		
116	TOTAL TOPOLOGICAL STATE 9	0.913	0.909		
117	TOTAL TOPOLOGICAL STATE 10	0.922	0.918		

FIG. 9E

LEAD	RANDOM	DIRECT	SISO/MISO	SISO/MISO	PC-MISO	PC-MISO
	SIMILARITY	SIMILARITY	SIMILARITY	IDENTITY	SIMILARITY	IDENTITY
1	1.754	0.480	0.501	69%	0.486	86%
2	1.158	0.238	0.279	56%	0.244	83%
3	1.664	0.655	0.680	64%	0.660	84%
4	1.291	0.179	0.213	60%	0.186	76%
5	1.763	0.327	0.335	82%	0.334	83%
6	1.196	0.201	0.224	58%	0.209	75%
7	1.294	0.274	0.291	72%	0.283	77%
8	1.385	0.268	0.288	73%	0.275	84%
9	1.694	0.464	0.481	74%	0.470	86%
10	1.613	0.460	0.470	79%	0.464	87%

FIG.10



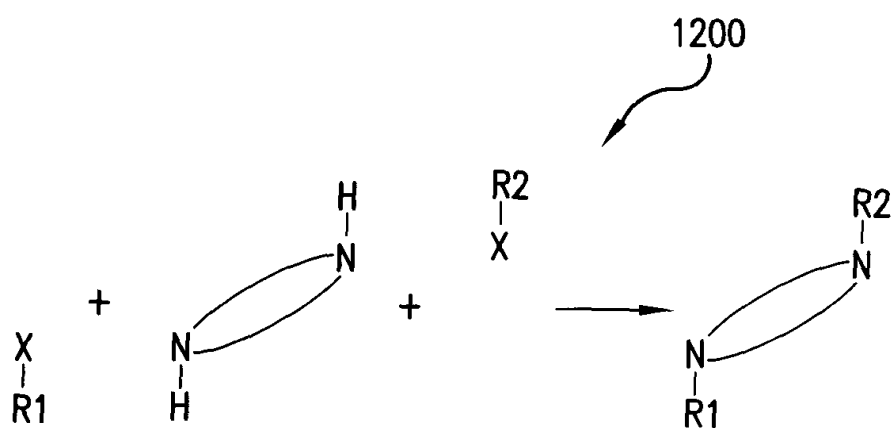


FIG. 12

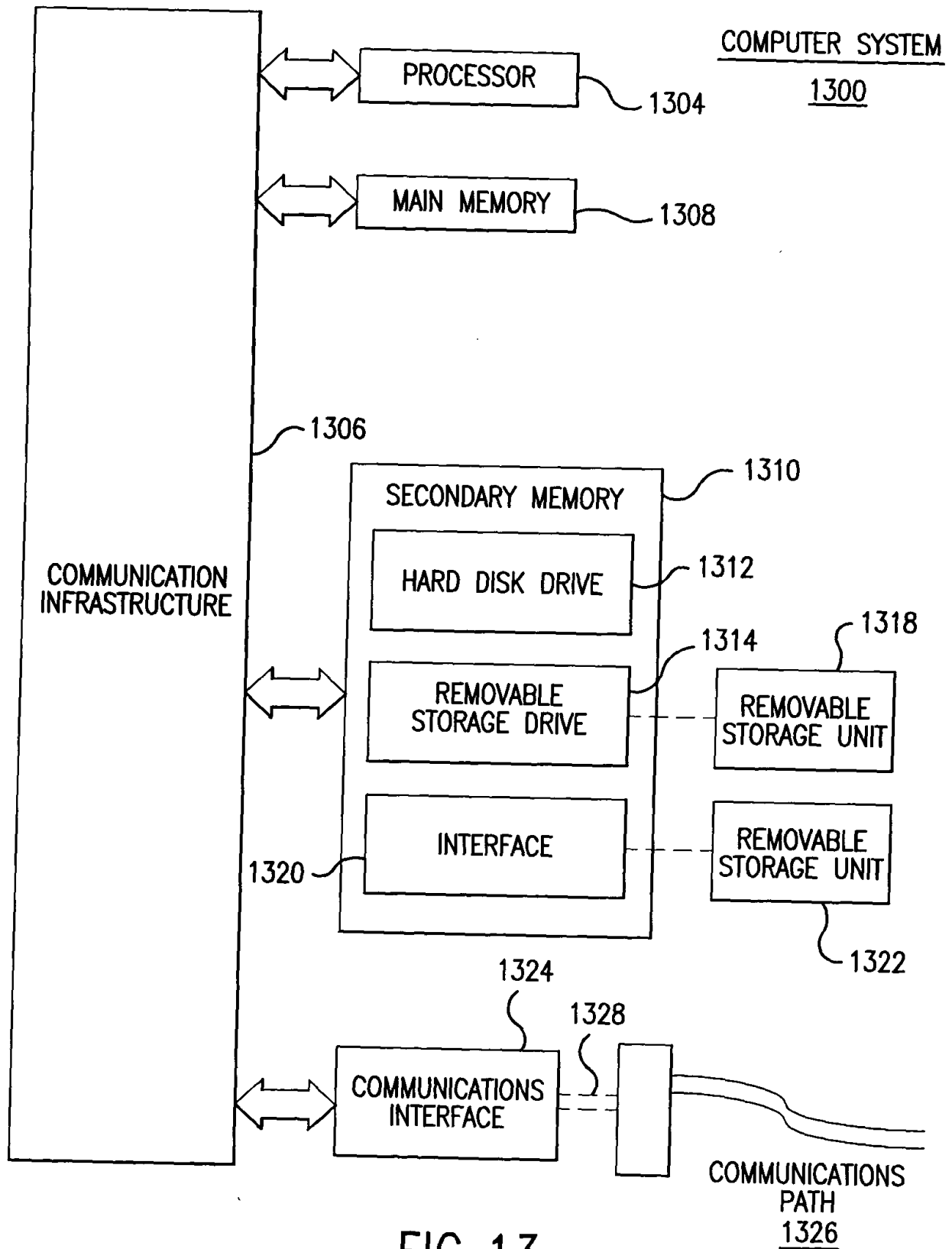


FIG. 13